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CCSI™

Carbon Capture Simulation Initiative

Validation and Uncertainty Quantification of Large scale CFD Models for Post Combustion Carbon Capture

Emily Ryan[1], William Lane[1], Curt Storlie[2], Chris Montgomery[3], Joanne Wendelberger[2]

[1]Department of Mechanical Engineering, Boston University, Boston, MA

[2]Los Alamos National Laboratory, Los Alamos, NM

[3]URS Corporation, Morgantown, WV

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U.S. DEPARTMENT OF ENERGY

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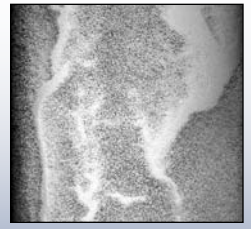
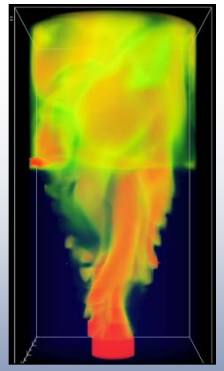


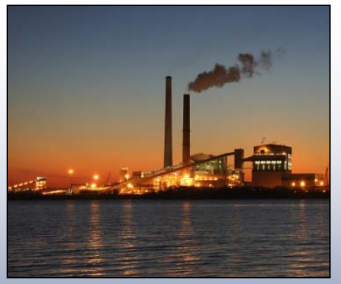

Identify promising concepts → **Reduce the time for design & troubleshooting** → **Quantify the technical risk, to enable reaching larger scales, earlier** → **Stabilize the cost during commercial deployment**

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- Institute for Clean and Secure Energy, The University of Utah

Industry

- Fluor
- B&W
- GE
- EPRI Electric Power Research Institute
- Air Products
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- URS
- Alstom
- Duke Energy
- Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
- Southern Company
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- Eastman

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Essential for accelerating commercial deployment

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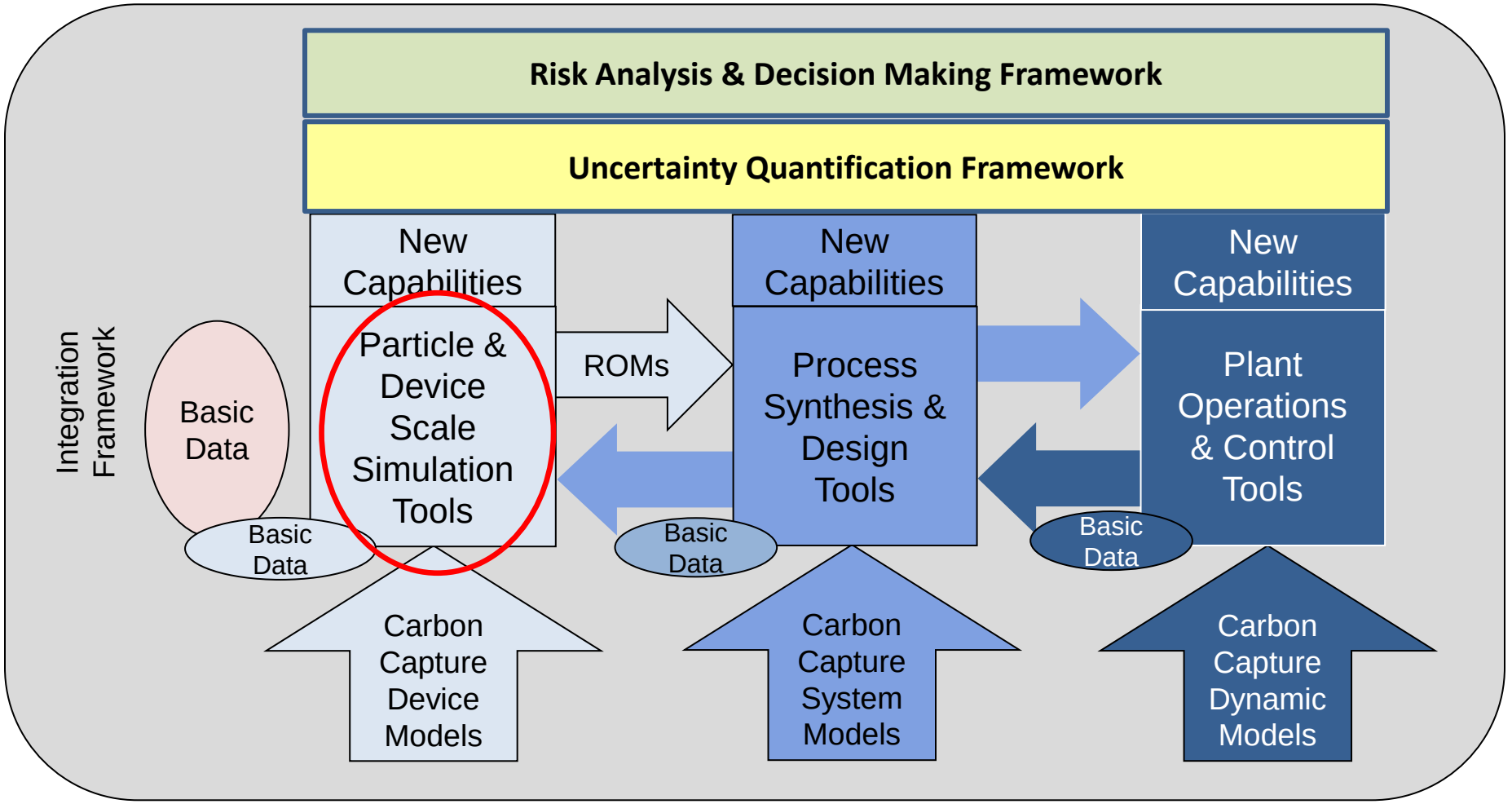
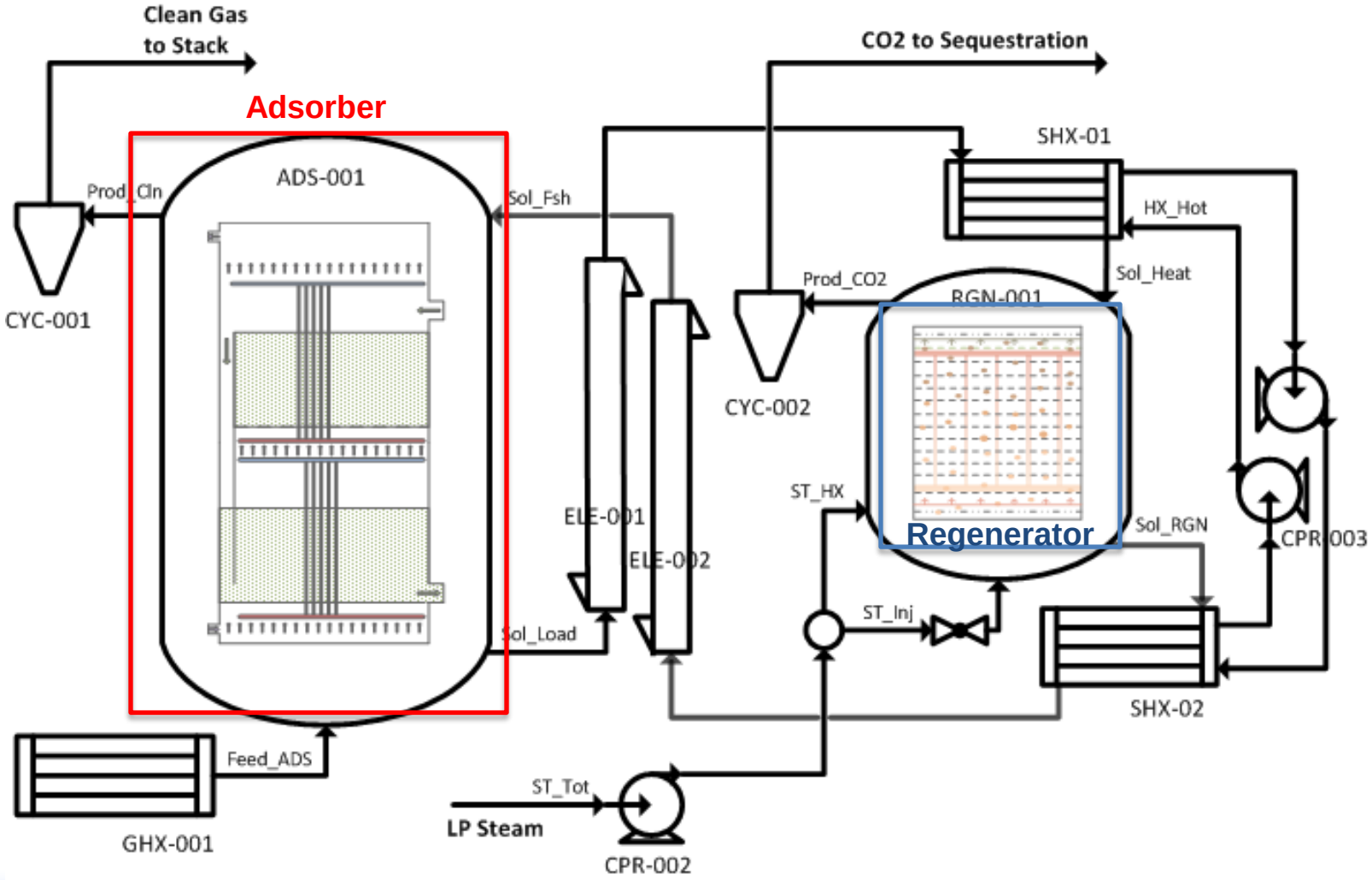
CCSI Toolset Overview



Overview of Particle and Device Scale Modeling

- Develop state-of-the-art device-scale simulation tools to accelerate the commercialization of carbon capture technologies.
  - Computational Fluid Dynamics (CFD) models of multi-phase circulating, bubbling and moving fluidized beds
  - Includes hydrodynamics, reactions and heat transfer of solid sorbent systems.
  - Quantify the accuracy of the CFD models by validating them with experimental data.
- Collaborate with other teams in CCSI to improve the design and performance of carbon capture technologies.
  - First principles modeling
  - Process level modeling
  - Uncertainty quantification
  - Reduced order model generation

Conceptual Full Scale CCSI Solid Sorbent Adsorber and Regenerator



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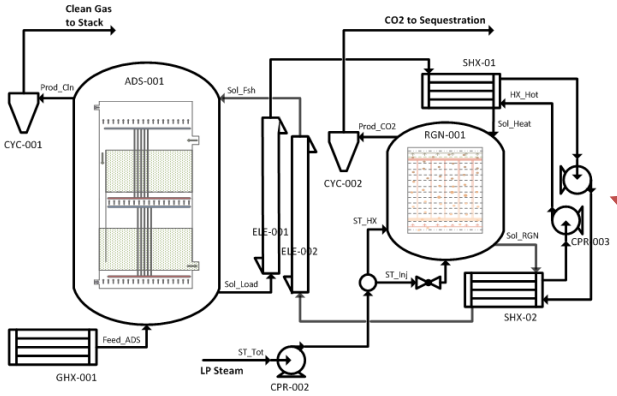
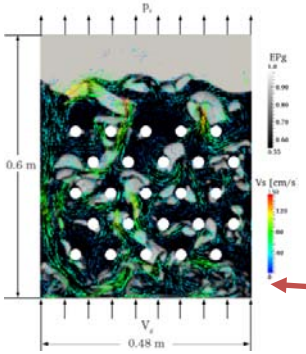
Validation and uncertainty analysis of CFD Models



Objective: To provide quantitative confidence on device-scale (CFD) model predictions for devices that are yet to be built.



CCSI CFD Validation Hierarchy

25 MWe, 100 MWe, 650 MWe Solid Sorbent Device Scale	Device Scale Systems
1 MWe ADA-ES Reactor	Pilot Scale Systems
NETL C2U/1 kW ADA-ES Reacting Moving Bed Unit: Bubbling Bed Adsorber; Moving Bed Regenerator	Laboratory Scale Subsystem (Coupled benchmark cases)
Intermediate Validation (Adsorber without reactions and heat transfer); Intermediate Validation (Regenerator without reactions and heat transfer)	Laboratory Scale Subsystem (Decoupled benchmark cases)
Upscaling (flow filtering); *Upscaling (reaction filtering)*; *Upscaling (energy filtering)*; *Upscaling (flow filtering)*	
Bubbling Fluidized Bed (Adsorber); Reaction Kinetic; Heat Transfer; Moving Fluidized Bed (Regenerator)	Unit Problems

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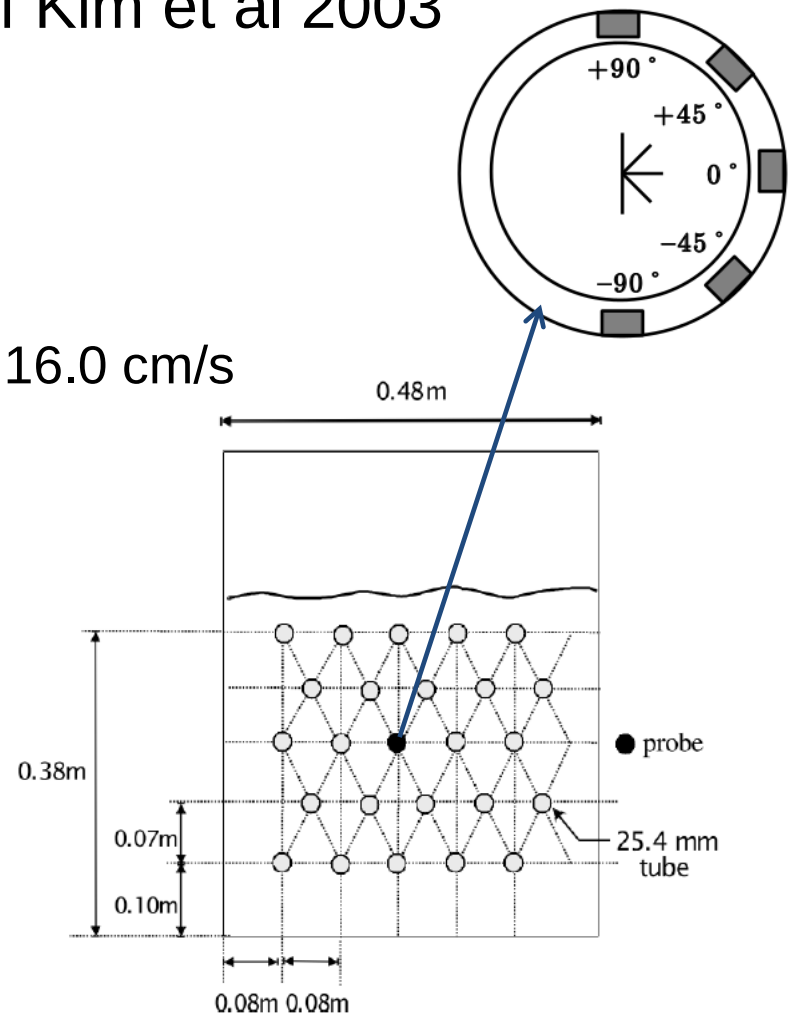
Bubbling Bed Unit Problem

- Initial validation/uncertainty quantification problem for CCSI
- Goals:
  - Develop framework for collaborations between UQ and CFD models
    - Communication between statisticians and engineers
    - Determine best methods for handling complex, slow CFD simulations
  - Validate bubbling bed model with experimental data
    - Determine the optimum model parameters for the BB model
    - Quantify our confidence in the model results

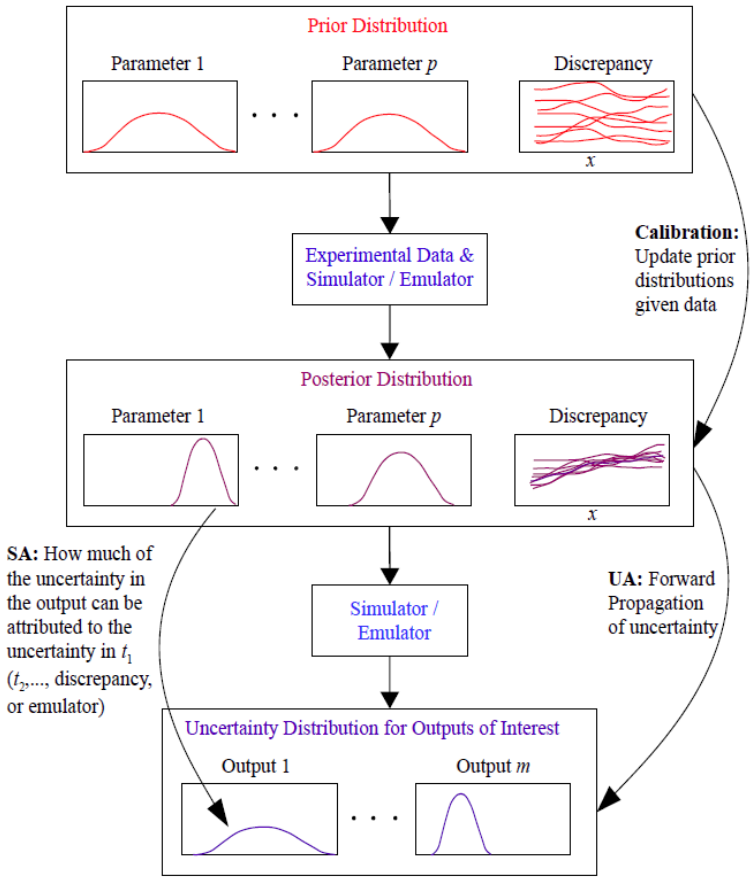
Bubbling Bed Setup

- Based on experimental setup of Kim et al 2003
- Setup
  - 0.34 x 0.48 x 0.60 m
  - Gas: air
    - Velocity = 5.5, 7.0, 11.0, 12.6, 16.0 cm/s
    - Pressure = 101.3 kPa
  - Solid: sand
    - Particle diameter = 240 μm
    - density = 2582 kg/m3
- Reported experimental results
  - Bubble frequency
  - Phase fraction



Uncertainty Quantification

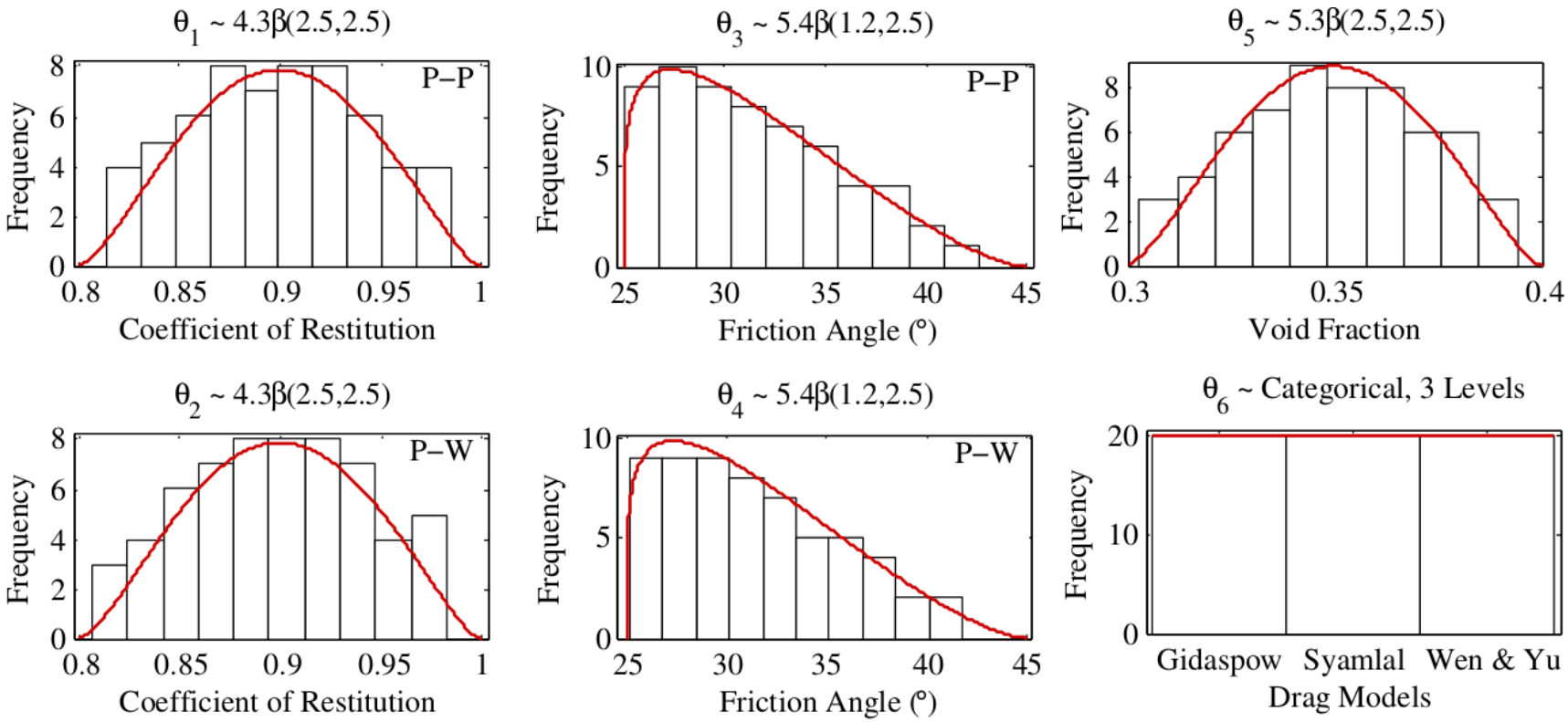
- Investigate effects of uncertain input parameters
  - Sensitivity analysis
  - Bayesian calibration
- Challenge: CFD simulations take 2 days to run
  - Not feasible to run 100-1000's of CFD simulations



Model Parameters

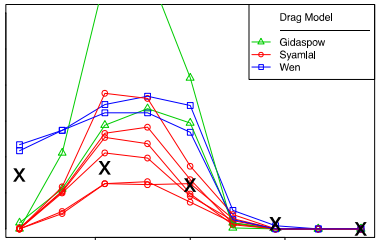
Parameters	**Range**	**Mode**
Continuous		
θ_1 = Coefficient of restitution, particle-particle (e_{pp})	0.8–0.997	0.9
θ_2 = Coefficient of restitution, particle-wall (e_{pw})	0.8–0.997	0.9
θ_3 = Friction angle, particle-particle (ϕ_{pp})	25.0–45.0	28.5
θ_4 = Friction angle, particle-wall (ϕ_{pw})	25.0–45.0	28.5
θ_5 = Packed bed void fraction (EP*)	0.3–0.4	0.35
Categorical	**Probability**	
θ_6 = Drag models (DM)		
Syamlal-O'Brien	33.4%	
Wen-Yu	33.3%	
Gidaspow	33.3%	

Prior Distribution of Model Parameters

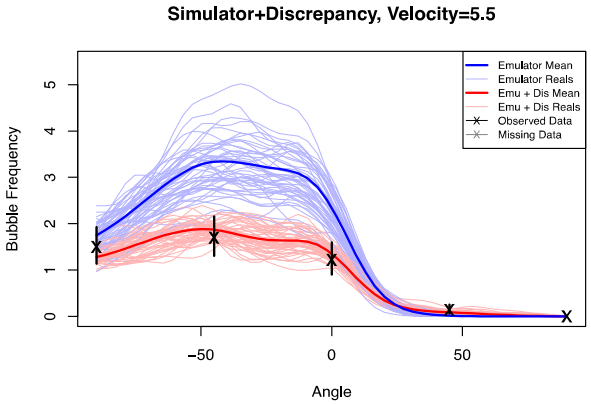


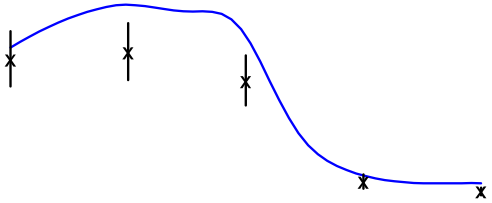
Calibration Process

- Latin Hypercube Sampling
  - Based on prior distributions
  - Setup 90 CFD runs
- CFD runs used to develop an emulator
  - Statistical model allows for 1000's of model runs
- Markov Chain Monte Carlo used to explore parameter space
  - Determine posterior distributions of model parameters



Emulator Results

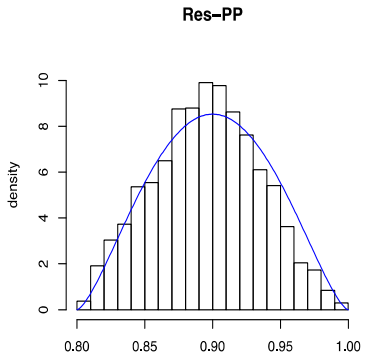


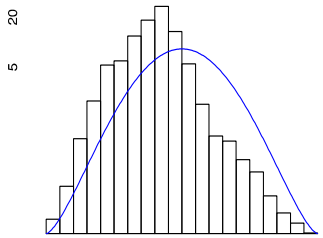


$$y_i = \eta(\mathbf{x}_i, \boldsymbol{\theta}) + \delta(\mathbf{x}_i) + \varepsilon_i$$

Results of Calibration Process

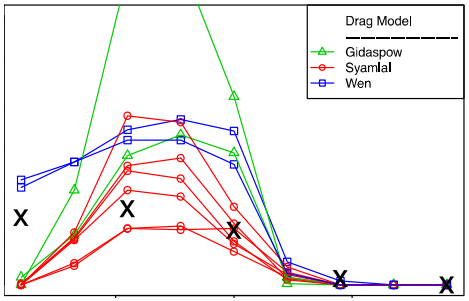
- Posterior distributions of model parameters
- Most model parameters did not change from prior distributions
  - Original values are appropriate
  - Not enough information in system to determine values
- Drag model greatly favored Wen-Yu
- Particle-Particle friction angel should be ~25°



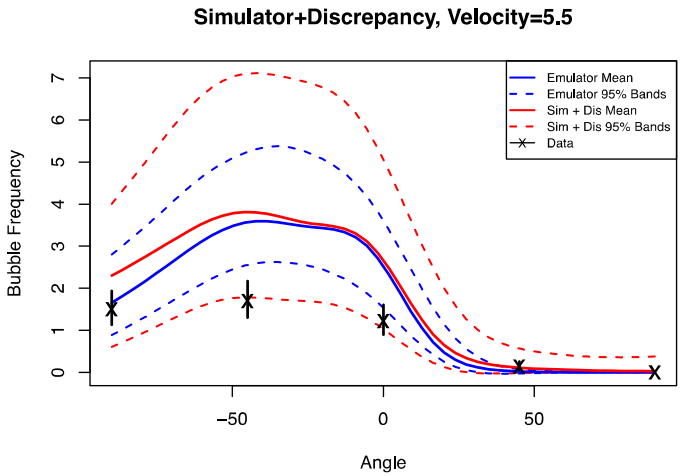


Drag Models and Fluidization

- Fluidization for system ~4.8 cm/s
- Near fluidization drag models are not valid
  - Gidaspow
  - Syamlal
- All drag models perform poorly at 5.5 cm/s



Cross Validation



Conclusions

- Developed methodology for combining CFD modeling and UQ for complex physical systems
- Results of model parameter studies will be used to investigate large systems and systems with different fluidization regimes
  - Is the calibrations done for the bubbling bed transferable to other systems
- Drag model selection can greatly affect results; especially near fluidization

Questions?

Contact information:
Emily Ryan
Boston University
ryanem@bu.edu

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